CHIN. PHYS. LETT. Vol. 26, No. 6 (2009) 060305

Partial Hermitian Conjugate Separability Criteria for Pure Quantum States *

ZHAO Xin(赵鑫)[1], WU Hua(吴华)[1], LI Yan-Song(李岩松)[1], LONG Gui-Lu(龙桂鲁)[1,2]**

[1]*Key Laboratory for Atomic and Molecular NanoSciences and Department of Physics, Tsinghua University, Beijing 100084*

[2]*National Laboratory for Information Science and Technology, Tsinghua University, Beijing 100084*

(Received 7 March 2009)

We propose a criterion for the separability of quantum pure states using the concept of a partial Hermitian conjugate. It is equivalent to the usual positive partial transposition criteria, with a simple physical interpretation.

PACS: 03.67.Hk, 03.65.Ud, 03.67.Dd

Entanglement and separability of quantum states has been an intriguing subject in quantum physics for a long time and has attracted much attention in recent years.[1−30] Several criteria have been proposed to examine the separability of quantum states. For pure states, the Schmidt decomposition[1,2,31] is a relatively simple method to determine the separability. For mixed states, however, the problem of separability becomes much more complicated. Bell inequalities[3,4] are among the earliest criteria able to test separability of this kind. They are necessary conditions for separability of bipartite quantum states. Recently many other criteria have also been put forward, among which the PPT criterion[5,6] is the most important one. This criterion was proved to be necessary and sufficient for separability in any 2×2 and 2×3 systems,[7] and it is only a necessary condition for systems of higher dimensions.

In this Letter, we introduce a criterion for the separability of bipartite pure states, the partial Hermitian conjugate (PHC) criterion. We then prove it to be a necessary and sufficient condition of separability for pure quantum states. The PPT criterion requires a partial transposition operation onto the density matrix of the system to be made, followed by an examination of the positivity of the newly acquired matrix. In our criterion, instead of the partial transposition operation, we need to make a partial Hermitian operation onto the density matrix of the system, then we compare the new matrix with the original density matrix. We prove that the system is separable if and only if the partial Hermitian conjugated matrix remains the same as the original density matrix.

First we explain the partial Hermitian conjugate operation. Suppose that a bipartite quantum system in a pure state is described by a vector

$$|\psi\rangle=\sum_{i,j}c_{ij}|ij\rangle, \tag{1}$$

with i,j representing the two sets of bases of the two subsystems, and c_{ij} the coefficient of $|ij\rangle$. If the state is separable, we can write the coefficients $c_{ij}=a_ib_j$, where a_i and b_j are the coefficients associated with $|i\rangle$, $|j\rangle$ respectively. That is,

$$|\psi\rangle=\sum_{i,j}a_ib_j|ij\rangle. \tag{2}$$

The density matrix of the entire system can then be written as

$$\rho=|\psi\rangle\langle\psi|=\sum_{i,j,i'j'}a_ib_ja_{i'}^*b_{j'}^*|ij\rangle\langle i'j'|. \tag{3}$$

We define the partial Hermitian conjugate of ρ as

$$\begin{aligned}\rho^{\rm PHC}&=\sum_{i,j,i'j'}a_ib_j^*a_{i'}^*b_{j'}|ij'\rangle\langle i'j|\\&=\sum_{i,j,i'j'}a_ib_{j'}a_{i'}^*b_j^*|ij'\rangle\langle i'j|.\end{aligned} \tag{4}$$

This means that we take an Hermitian conjugate operation on the second subsystem: exchange the index of the bases of the second subsystem in $|\psi\rangle$ and $\langle\psi|$, then take the conjugate of the coefficients of the second subsystem.

The partial Hermitian conjugate criterion: $|\psi\rangle$ is separable if and only if $\rho^{\rm PHC}=\rho$.

Now we prove this criterion. The necessity is obvious. If $|\psi\rangle$ is separable, then $|\psi\rangle$ can be written in the form

$$|\psi\rangle=\sum_i a_i|i\rangle\otimes\sum_j b_j|j\rangle, \tag{5}$$

the density matrix

$$\begin{aligned}\rho=|\psi\rangle\langle\psi|&=\sum_{i,i'}a_ia_{i'}^*|i\rangle\langle i'|\otimes\sum_{j,j'}b_jb_{j'}^*|j\rangle\langle j'|\\&=\rho_a\otimes\rho_b.\end{aligned} \tag{6}$$

*Supported by the National Natural Science Foundation of China under Grant Nos 10775076 and 10874098, the National Basic Research Program of China under Grant Nos 2006CB921106 and 2009CB929402, the Specialized Research Fund for the Doctoral Program of Education Ministry of China under Grant No 20060003048.

**To whom correspondence should be addressed. Email: gllong@tsinghua.edu.cn

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where ρ can be written as the outer vector product of the density matrices of the two subsystems ρ_a and ρ_b. In this case, the partial Hermitian conjugate of ρ is

$$\begin{aligned}\rho^{\rm PHC} &= \left(\sum_i a_i|i\rangle \otimes \sum_{j'} b_{j'}|j'\rangle\right) \\ &\quad \cdot \left(\sum_{i'} a^*_{i'}\langle i'| \otimes \sum_j b^*_j\langle j|\right) \\ &= \sum_{i,i'} a_i a^*_{i'}|i\rangle\langle i'| \otimes \sum_{j',j} b_{j'} b^*_j |j'\rangle\langle j| \\ &= \rho_a \otimes \rho_b^\dagger. \end{aligned} \tag{7}$$

As ρ_b is a density matrix, we can prove that $\rho_b^\dagger = \rho_b$, so we have

$$\rho^{\rm PHC} = \rho. \tag{8}$$

To show the sufficiency, we must prove that if a pure state quantum system with density matrix ρ has the property $\rho^{\rm PHC} = \rho$, then the system is separable. However, for a general bipartite state, it is unclear how to define the PHC operation. Unlike the partial transposition operation where only index exchanges are performed, the PHC also needs complex conjugation on the coefficients. This complex conjugate is not defined uniquely because in the product $c_{i,j} = a_i b_j$ one can always shift something to a_i, the first particle, and then divide it out in b_j, the second particle. For instance, $1/2$ can be either written as $1/\sqrt{2} \times 1/\sqrt{2}$ or written as $i/\sqrt{2} \times (-i)/\sqrt{2}$ or $(-i)/\sqrt{2} \times i/\sqrt{2}$. To overcome this difficulty, we first make a unitary transformation to write the state in the Schmidt basis. In the Schmidt basis, the PHC is defined clearly. Then we make the PHC in the Schmidt basis and then transform back to the original basis.

We now define the PHC in the Schmidt basis. According to the theorem of Schmidt decomposition, any bipartite pure state $|\psi\rangle$ can be written as

$$|\psi_S\rangle = \sum_i \lambda_i |ii'\rangle, \tag{9}$$

where λ_i are real numbers, $|i\rangle, |i'\rangle$ are Schmidt bases of the two subsystems. Note that i and i' are not independent, therefore the summation is over the i index only. Then the density matrix

$$\rho_S = \sum_{i,j} \lambda_i \lambda_j |ii'\rangle\langle jj'|, \tag{10}$$

and its partial Hermitian conjugation is

$$\rho_S^{\rm PHC} = \sum_{i,j} \lambda_i \lambda_j |ij'\rangle\langle ji'|, \tag{11}$$

which is clear and operational.

The sufficiency of the PHC criterion is clear. If $\rho_S^{\rm PHC} = \rho_S$, then

$$\sum_{i,j} \lambda_i \lambda_j |ii'\rangle\langle jj'| = \sum_{i,j} \lambda_i \lambda_j |ij'\rangle\langle ji'|, \tag{12}$$

i.e. for any i, j, if $\lambda_i \lambda_j \neq 0$, there must be

$$|ii'\rangle\langle jj'| = |ij'\rangle\langle ji'|, \tag{13}$$

which is impossible for any $i \neq j$. Thus the only possibility is $i = j = 1$, the Schmidt decomposition of $|\psi\rangle$ has only one non-zero Schmidt coefficient λ_1. A pure state is separable if its Schmidt decomposition has only one non-zero Schmidt coefficient.[15] Therefore $|\psi\rangle$ is separable, it can be written as the outer vector product of the states of the two subsystem $|\psi\rangle = \lambda_1 |1\rangle \otimes |1'\rangle$.

Now that we have proved sufficiency in the Schmidt bases, if $|\psi_S\rangle$ satisfies $\rho_S^{\rm PHC} = \rho_S$, then it is separable. We continue to prove it in arbitrary bases. Suppose a pure state $|\psi_S\rangle = \sum_i \lambda_i |i\rangle \otimes |i'\rangle$ written in the Schmidt decomposition bases satisfies $\rho_S^{\rm PHC} = \rho_S$. U is the transformation matrix between the bases of Schmidt decomposition and any other bases. Since U is a unitary and local transformation, then we can write U as the outer product of the transformation matrices of the two subsystems $U = U_a \otimes U_b$, which can be worked out using standard procedure in the Schmidt decomposition theorem.[1,2,31] In the new bases, the state is written as

$$|\psi\rangle = U|\psi_S\rangle = \sum_i \lambda_i U_a |i\rangle \otimes U_b |i'\rangle, \tag{14}$$

the density matrix is

$$\begin{aligned}\rho &= U|\psi_S\rangle\langle\psi_S|U^\dagger \\ &= \sum_{i,j} \lambda_i \lambda_j U_a |i\rangle\langle j| U_a^\dagger \otimes U_b |i'\rangle\langle j'| U_b^\dagger, \end{aligned} \tag{15}$$

the partial Hermitian conjugation is

$$\rho^{\rm PHC} = \sum_{i,j} \lambda_i \lambda_j U_a |i\rangle\langle j| U_a^\dagger \otimes U_b^\dagger |j'\rangle\langle i'| U_b. \tag{16}$$

Writing U_b in matrix element form, we have

$$\rho = \sum_{i,j} \lambda_i \lambda_j U_a |i\rangle\langle j| U_a^\dagger \otimes \left(\sum_{k,l} u_{b,ki} |k'\rangle\langle l'| u^*_{b,lj}\right), \tag{17}$$

the partial Hermitian conjugation is then

$$\rho^{\rm PHC} = \sum_{i,j} \lambda_i \lambda_j U_a |i\rangle\langle j| U_a^\dagger \otimes \left(\sum_{k,l} u^*_{b,lj} |k'\rangle\langle l'| u_{b,ki}\right). \tag{18}$$

Equation (18) is the definition of PHC operation for an arbitrary bipartite pure state.

Now it is easy to show that under such a definition, if the state is invariant under PHC, then it is separable. From the definition of PHC for a general bipartite pure state, if $\rho^{\rm PHC} = \rho$, then we can reach $\rho_S^{\rm PHC} = \rho_S$. Thus from the Schmidt criterion, the state is separable.

Therefore, we prove that any pure state which has $\rho^{\rm PHC} = \rho$ is separable. Together with the necessity proved earlier in this study, we prove that $\rho^{\rm PHC} = \rho$ is a necessary and sufficient condition of separability of any pure state. Here we give the PHC for the second particle, and the PHC with respect to the first particle can also be likewise defined. In a pure multipartite quantum system, the PHC with respect to a specific particle can also be similarly worked out by treating the remaining particles as a single particle.

However, we must notice that this criterion cannot be generalized to mixed states. Of course, $\rho^{\rm PHC} = \rho$ is always a necessary condition for separability for mixed state, but it is not a sufficient condition.

Now we give some examples of the application of the criterion. Suppose the state $|\psi\rangle = \frac{1}{2}(|00\rangle + i|01\rangle + i|10\rangle - |11\rangle)$; we know that it is separable $|\psi\rangle = \frac{1}{2}(|0\rangle + i|1\rangle)(|0\rangle + i|1\rangle)$. Its density matrix is

$$\rho = \frac{1}{4}\begin{pmatrix} 1 & -i & -i & -1 \\ i & 1 & 1 & -i \\ i & 1 & 1 & -i \\ -1 & i & i & 1 \end{pmatrix}, \tag{19}$$

and the partial Hermitian conjugate matrix (the Hermitian conjugation operation is made on the second subsystem) is the same, $\rho^{\rm PHC} = \rho$.

Consider another pure state $|\psi\rangle = \frac{1}{2}(|00\rangle + i|01\rangle + |10\rangle + |11\rangle)$. The density matrix is

$$\rho = \frac{1}{4}\begin{pmatrix} 1 & -i & 1 & 1 \\ i & 1 & i & i \\ 1 & -i & 1 & 1 \\ 1 & -i & 1 & 1 \end{pmatrix}. \tag{20}$$

Through some calculations, we obtain the partial Hermitian conjugate matrix (the operation is made on the second subsystem)

$$\rho^{\rm PHC} = \frac{1}{4}\begin{pmatrix} 1 & -i & i & 1 \\ i & 1 & i & 1 \\ -i & -i & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}, \tag{21}$$

so $\rho^{\rm PHC} \neq \rho$, $|\psi\rangle$ is inseparable.

Operationally, the PHC separability criterion is equivalent to the Schmidt criterion, because the PHC operation needs the calculation of Schmidt decomposition. However, the PHC criterion has a clear physical interpretation: when a pure quantum state is separable, a partial Hermitian conjugate on a specific particle will leave the quantum state unchanged. The PPT criterion is also a necessary and sufficient condition for pure quantum states; the physical interpretation of the PPT criterion is that the partially transposed density matrix is still a density matrix if the state is separable. Though the PHC criterion does not lend us more convenience, it leads us to consider the separability problem from a different angle. In addition, the PHC criterion may provide a new tool to quantitatively describe entanglement. For instance, one application of the PHC criterion is to use the departure of the PHC density matrix from its original density matrix as a measure of entanglement. This is an interesting subject and is under study right now.

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